Brief report on theoretical research upon wood thermal property

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Abstract: In this paper, the theoretical expressions of the specific heat and thermal conductivity of wood are first derived from the micro-structure of wood by applying some basic principles in statistical thermodynamics and physical mechanics. Tested by a great many experiments, the average error of theoretical values is about 5%, much less than that of all kinds of exiting empiric equations in the world.

Key words: Specific heat; thermal conductivity; theoretical expression; Wood

CLC number: S781.37 **Document code:** A **Article ID:** 10007-662X(2000)02-0145-02

Introduction

Thermal properties of wood such as specific heat, thermal conductivity and so on are parameters which is required in scientific research and heat treatment of wood. Because wood is a kind of natural polymer organism whose chemical element and microstructure are very complicated, it's very difficult to study its thermal property theoretically, therefore, for almost one century, it was by means of experiment that the scientists at home and abroad studied the thermal property of wood directly (Dunlap 1912; Kollmann 1968; Cheng 1985; Gao 1985; Zhang 1986) But the question is that the empiric equations of the wood thermal property derived from experimental data by means of mathematical fitting have different functions, and different adaptable area (species tress, moisture content, temperature and so on), with a larger error, lacking the theoretical foundation. In order to solve the above-mentioned problems, the universal theoretical expressions of wood thermal property are derived in this paper by means of basic principles of various natural subjects, such as statistical mechanics, physical mechanics, wood physics etc.

Theoretical expression of wood specific heat

The theoretical model to develop specific heat of wood is based on cell structure of wood, that is, the pyran-rings, the basic unit of wood cellulose, are connected into a long-chain high polymer by glucose linkages. One pyran-ring has 20 atoms, 60 degrees of freedom, among which 54 degrees are of internal vibration including the stretching and bending vibration of C-C, C-H, C-O, O-H bonds, and they all belong to the Einstein's mode of vibration. As to the other six, three of them are of translation freedom in the mass center of pyran-ring, the other three are of rotary freedom. These six degrees of freedom belong to the Debye's mode of vibration. There are also oxygen atoms among rings, because the mass of oxygen atom between two rings is far below the whole mass of the atoms in the ring, it can't form Debye's mode of vibration. So these three degrees of freedom belong to the Einstein's mode of vibration too. Therefore, the theoretical expression of specific heat of dry wood is given as:

$$C_0(T)=\frac{R}{\mu}\left[6D\left(\frac{\Theta_D}{T}\right)+\sum_{\nu=1}^{57}\frac{(\Theta_\nu/2T)^2}{\sinh^2(\Theta_\nu/2T)}\right] \quad (1)$$

where Θ_D and $D\left(\frac{\Theta_D}{T}\right)$ are called Debye's characteristic temperature and Debye function respectively, and Θ_ν is the characteristic temperature of each chemical bond among rings, R is universal constant of gases, μ is molar mass of the glucose group.

In order to simplify calculation, we can expand expression (1) into Taylor series at T=273.15K, then, by substituting known quantity, we can obtain

$$C_0(t) = 1.2294 + 0.006714\, t \quad (\mathrm{kJ \cdot kg^{-1} \cdot K^{-1}}) \quad (2)$$

It is obvious that there is a simple relationship between the specific heat of dried wood C_0 and that of the wet wood C_w (whose moisture content is w%):

Foundation item: This paper is part of Theoretical Research on Wood Thermal Property which is supported by Natural Science Foundation of Fujian Province.

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Received date: 2000-03-30

Responsible editor: Chai Ruihai

$$C_w = \frac{C_0 + C' \cdot w\%}{1 + w\%} \tag{3}$$

Where C' is the specific heat of water.

We calculate the specific heat of 33 species of wood with different moisture contents and temperatures by means of equations (2) and (3). When the theoretical values are compared with the experimental values in the same conditions, it has been discovered that the maximum error is 7.8%, and the average error is 2.5%.

Theoretical expressions of thermal conductivity of wood

In order to derive the theoretical expression of thermal conductivity of wood, we shall assume that the phonon is the carrier of energy in heat conduction of wood. The phonon shows the particle property of lattice wave, and move irregularly in all directions in wood at sound velocity of u as gas molecules do, colliding each other and exchanging their energy. A phonon with velocity u, total energy E and mean free path L can transport energy E when it passes through the distance of L.

Considering the double direction movement of various phonons, we find that energy is transported from the region of larger E to the one of smaller E, that is, from the region with higher temperature to the region with lower temperature. We can thus derive the theoretical expression of thermal conductivity of dry wood, and find

$$\lambda_0 = \frac{R}{M} \rho u L D\left(\frac{\Theta_D}{T}\right) \tag{4}$$

Where M is molar mass of wood cell, ρ is mass density of dry wood, and other sings mean the same as stated above.

The mean free path of the phonon L is related not only to the direction of heat current, but also to the frequency of sound wave in wood, temperature and density of wood, etc. Therefore, it is very difficult to decide the expression of the mean free path L of the phonon theoretically. According to the experimental results and theoretical analysis. We assume that there exists the relationship between the mean free path L and temperature T density of wood, Debye characteristic temperature Θ_D as follows.

$$L = C_1 \left(\frac{T}{\Theta_D}\right)^{3/2} \exp\left(C_2 \sqrt{\frac{\rho_A}{\rho}}\right) \tag{5}$$

Where ρ_A is density of air (values in normal state), C_1 and C_2 are two constants to be decided. (C_1 is of length's dimension) and can be decided according to the experimental data of the thermal conductivity. On the basis of better accuracy, we can use C_1=10.15×10^{-10} m, C_2=7.987 (for heat current in the choral direction), and C_1=12.60×10^{-10} m, C_2=5.283 (for heat current in the radical direction).

In order to simplify calculation, we can expand expression (4) into Taylor's series at T=273.15K, and expand $T^{3/2}$ in expression (5) into power series of t. Then, by substituting known quantity, we can obtain separately simplified formula of wood thermal conductivity in the choral and radial direction.

$$\lambda_{cho} = (9.257 + 0.0519t) \times 10^{-3} \frac{\rho}{\sqrt{u}} \exp\left(\frac{9.027}{\sqrt{\rho}}\right) \quad \left(W \cdot m^{-1} \cdot K^{-1}\right) \tag{6}$$

$$\lambda_{rad} = (11.49 + 0.0645t) \times 10^{-3} \frac{\rho}{\sqrt{u}} \exp\left(\frac{6.0}{\sqrt{\rho}}\right) \quad \left(W \cdot m^{-1} \cdot K^{-1}\right) \tag{7}$$

The relationship between thermal conductivity of dried wood and that of wet wood (whose moisture content is w%) is shown as the following equation

$$\lambda_w = (1 + 1.25w\%)\lambda_0 \tag{8}$$

We have calculated the thermal conductivity of 23 species of wood in choral direction and that of 18 species of wood in radial direction. It is easy to see that the maximum error of the former is 11.9% and that of the latter 13.7%, and the average error of the former is 4.8% and that of latter 5.3%, as the theoretical values is compared with the experimental values.

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